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Starting Algorithms for Gauss Runge-Kutta Methods for Hamiltonian Systems

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Abstract—Among the symplectic integrators for the numerical solution of general Hamiltonian systems, implicit Runge-Kutta methods of Gauss type (RKG) play an important role. To improve the efficiency of the algorithms to be used in the solution of the nonlinear equations of stages, accurate starting values for the iterative process are required. In this paper, a class of starting algorithms, which are based on numerical information computed in two previous steps, is studied. For two- and three-stages RKG methods, explicit starting algorithms for the stage equations with orders three and four are derived. Finally, some numerical experiments comparing the behaviour of the new starting algorithms with the standard first iterant based on Lagrange interpolation of stages in the previous step are presented.

Keywords—Starting algorithms, Runge-Kutta, Gauss methods, Hamiltonian systems.

1. INTRODUCTION

Implicit Runge-Kutta methods of Gauss type (RKG), also called Kuntzmann-Butcher methods, have been the subject of many studies due mainly to their high order and good stability properties. In addition, recent studies show that these methods play an essential role in connection with the so-called "geometric integration". In fact, as shown by Sanz-Serna and Calvo [1], RKG methods with constant step sizes are symplectic integrators, i.e., preserve the symplectic structure of space phase for arbitrary Hamiltonian functions. Furthermore, in order to use variable step sizes, it has been proved independently by Hairer [2] and Reich [3] that the so-called Poincaré transformation allows us to introduce a step-size function which controls the size of the step dynamically and retains the Hamiltonian character of the differential equations. However, some separable Hamiltonians may loose such separability in this regularization process (e.g., the two-body problem with the eccentric or true anomalies), and therefore, only symplectic methods for general Hamiltonians such as RKG methods can be used in this variable step-size setting.

On the other hand, RKG methods have been used in connection with other geometric integrators such as reversible integrators [4] in which an involution ρ of the exact flow is preserved also by the numerical integrators. In conclusion, RKG methods, in spite of their implicitness, are good potential candidates for geometric integration since they retain all the advantages of symplectic integrators even in a variable stepsize integration based on a Poincaré regularization technique. Recall that as shown by Calvo, Lopez-Marcos and Sanz-Serna [5], this approach has some advantages over other existing variable step-size techniques.

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The purpose of this paper is to construct starting algorithms which do not require additional function evaluations for the iterative solution of the implicit equation of stages by using the available information of two previous steps for the two- and the three-step RKG methods. It must be recalled that a similar approach (but by using the available information of one step) was studied by one of the authors (Laburta [6,7]) obtaining explicitly starting algorithms for several implicit Runge-Kutta methods. The paper is organized as follows. In Section 2, after introducing the basic notations, some basic facts of Butcher series have been used to derive the order conditions of the starting algorithms. Section 3 deals with the two stage RKG method. Here, a family of third-order starting algorithms depending on a free parameter is derived. Then, taking into account the fourth-order conditions, three algorithms corresponding to different choices of the free parameter are derived. In Section 4, starting algorithms for the three-stage RKG method are considered. It is found that there exists a two parameter family of fourth-order starting algorithms such that any of them cannot attain order five. Then these available parameters have been chosen taking into account the coefficients of the error terms of orders five and six. Finally, in Section 5, the results of some numerical experiments comparing the new starting algorithms with the standard algorithm based on Lagrange interpolation of stages in the previous step are presented. It is concluded that, compared with the standard one, the new algorithms are more robust and reduce (on average) the number of fixed-point iterations by one without requiring additional function evaluations.

2. ORDER CONDITIONS FOR LINEAR TWO-STEP STARTING ALGORITHMS

Let us suppose than an implicit s-stage Runge-Kutta (RK) method defined by the coefficients $A = (a_{ij}) \in \mathbb{R}^{s\times s}$, $b = (b_i) \in \mathbb{R}^s$ is applied to the autonomous initial value problem

$$\begin{aligned} y'(t) &= f(y(t)), \qquad t \in [t_0, t_0 + T], \\ y(t_0) &= y_0 \in \mathbb{R}. \end{aligned} \tag{1}$$

To simplify the presentation, we assume that (1) is a scalar differential system, that matrix A of the RK method is a nonsingular matrix, and also that the integration advances with a fixed step size denoted by h.

If we denote by y_n the approximation to the solution of (1) at the grid point t_n, the equations of the RK method (A, b) that advances from (t_n, y_n) to (t_{n+1}, y_{n+1}) are

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(Y_{n,i}),$$

where the so-called (internal) stages $Y_{n,i}$, $(i = 1, \ldots, s)$ are computed from the implicit equations

$$Y_{n,i} = y_n + h\sum_{j=1}^{s} a_{ij} f(Y_{n,j}), \qquad (i = 1, \ldots, s). \tag{2}$$

In order to solve iteratively these implicit equations, accurate starting values $Y_{n,i}^{(0)}$, $(i = 1, \ldots, s)$ to the exact solution of (2) are desirable. Hence, our aim is to derive starting algorithms that provide accurate starting values with minimal computational cost, i.e., by using quantities that have been computed in two previous steps.

Since we are using numerical information from two previous steps, we will assume that we are advancing from $t_{n+1} \to t_{n+2}$, and therefore, our algorithm will use information of steps $t_{n-1} \to t_n$ and $t_n \to t_{n+1}$. Denoting by $Y_{n+1,i}^{(0)}$ $(i = 1, \ldots, s)$ the initial approximations to the stages $Y_{n+1,i}$, we will consider starting algorithms of the following type:

$$Y_{n+1,i}^{(0)} = \alpha_i y_{n-1} + \sum_{j=1}^{s} \left[\beta_{i,j} Y_{n-1,j} + \gamma_{i,j} Y_{n,j}\right], \qquad (i = 1, \ldots, s), \tag{3}$$

where α_i, $\beta_{i,j}$, and $\gamma_{i,j}$ are constants that will be determined taking into account the accuracy of $Y^{(0)}_{n+1,i}$ with respect to $Y_{n+1,i}$.

Introducing the vector notations

$$\begin{aligned}\beta_i^\top &= (\beta_{i,1}, \beta_{i,2}, \ldots, \beta_{i,s}) \in \mathbb{R}^s,\\ \gamma_i^\top &= (\gamma_{i,1}, \gamma_{i,2}, \ldots, \gamma_{i,s}) \in \mathbb{R}^s,\\ Y_l &= (Y_{l,1}, Y_{l,2}, \ldots, Y_{l,s})^\top \in \mathbb{R}^{sm},\end{aligned}$$

equations (3) can be written in the vector form

$$Y^{(0)}_{n+1,i} = \alpha_i y_{n-1} + \beta_i^\top Y_{n-1} + \gamma_i^\top Y_n, \qquad (i = 1, \ldots, s). \tag{4}$$

It must be noticed that (4) defines the approximation $Y^{(0)}_{n+1,i}$ as a linear combination of stages in the two previous steps and y_{n-1}, but this back value can be substituted by y_{n+1} and we have an equivalent algorithm. In fact, by introducing the vector $d \in \mathbb{R}^s$ such that $d^\top = b^\top A^{-1}$ and the scalar $\mu = 1 - d^\top e \neq 0$, the equations that advance the two previous steps can be written in terms of stages as

$$y_{j+1} = \mu y_j + d^\top Y_j, \qquad j = n, \quad n-1,$$

and therefore,

$$y_{n-1} = \mu^{-2} y_{n+1} - \mu^{-2} d^\top Y_n - \mu^{-1} d^\top Y_{n-1}. \tag{5}$$

Hence, by substituting (5) into the right-hand side of (4) we arrive at

$$Y^{(0)}_{n+1,i} = \mu^{-2}\left[\alpha_i y_{n+1} + \left(\mu^2\beta_i - \mu\alpha_i d\right)^\top Y_{n-1} + \left(\mu^2\gamma_i - \alpha_i d\right)^\top Y_n\right], \tag{6}$$

which is equivalent to (4). Although the starting algorithm in form (4) will be used in our study of the order conditions, the last equivalent expression (6) will be employed in our numerical experiments because it uses the most recent value y_{n+1} instead of the back value y_{n-1}.

To obtain the power series expansion of $Y_{n+1,i}$ at the point y_{n-1} with respect to the step size h, observe that the exact stages can be considered as the result of a $(3s)$-stage Runge-Kutta type algorithm defined by the Butcher array

$$\begin{array}{c|c} \tilde{c} & \tilde{A} \\ \hline & \tilde{b}_i^\top \end{array} = \begin{array}{c|ccc} c & A & 0 & 0 \\ e+c & eb^\top & A & 0 \\ 2e+c & eb^\top & eb^\top & A \\ \hline & b^\top & b^\top & A_i^\top \end{array}$$

where $c = Ae \in \mathbb{R}^s$ with $e = (1, \ldots, 1)^\top \in \mathbb{R}^s$ and $A_i^\top$ is the i^{th} row of A. Hence, by using the theory of the Butcher's series (B-series) (see [8, Theorem 2.11]), we can write

$$Y_{n+1,i} = y_{n-1} + \sum_{\substack{\tau \in T \\ \rho(\tau) \geq 1}} \frac{\alpha(\tau)\gamma(\tau)}{\rho(\tau)!} \left(\tilde{b}_i^\top \tilde{\Phi}(\tau)\right) \mathbf{f}(\tau)(y_{n-1}) h^{\rho(\tau)}, \qquad (i = 1, \ldots, s). \tag{7}$$

Here, T denotes the set of the rooted trees, $\alpha(\tau)$, $\gamma(\tau)$, and $\rho(\tau)$ are real-valued functions defined on the set T which represent the number of the monotonic labellings, the density, and the order of τ, respectively. The vector function $\mathbf{f}(\tau)(y_{n-1}) \in \mathbb{R}^m$ is the elementary differential of f corresponding to the tree τ evaluated at y_{n-1}, and $\tilde{\Phi} : T \to \mathbb{R}^{3s}$ is the elementary weight function associated to the matrix $\tilde{A}$ of the above tableau.

For the power series expansion of (4) at y_{n-1}, we observe first that Y_{n-1}, Y_n can be considered as the $2s$ stages associated to the matrix

$$\bar{A} = \begin{pmatrix} A & 0 \\ eb^\top & A \end{pmatrix},$$

starting from y_{n-1} with step size h. On the other hand, using the stage functions

$$F(Y_k) = (f(Y_{k,1}), \ldots, f(Y_{k,s}))^\top,$$

and taking into account the stage equations in the steps $t_{n-1} \to t_n$ and $t_n \to t_{n+1}$, the right-hand side of (4) can be written in the form

$$Y^{(0)}_{n+1,i} = \left(\alpha_i + \beta_i^\top e + \gamma_i^\top e\right) y_{n-1} + h\left(\beta_i^\top, \gamma_i^\top\right) \bar{A} \begin{pmatrix} F(Y_{n-1}) \\ F(Y_n) \end{pmatrix}.$$

Then, assuming the consistency conditions

$$\alpha_i + \beta_i^\top e + \gamma_i^\top e = 1, \qquad i = 1, \ldots, s, \tag{8}$$

the approximation to the i^{th} stage $Y^{(0)}_{n+1,i}$ can be considered as the result to apply a $2s$-stage RK scheme defined by $\bar{A}$ and $\bar{b}_i^\top = (\beta_i^\top, \gamma_i^\top)\bar{A} \in \mathbb{R}^{2s}$ to the differential equation $y' = f(y)$ at y_{n-1} with step size h. Hence, denoting by $\bar{\Phi}(\tau) \in \mathbb{R}^{2s}$ the elementary weight function associated to the $2s$ matrix $\bar{A}$, we have

$$Y^{(0)}_{n+1,i} = y_{n-1} + \sum_{\substack{\tau \in T \\ \rho(\tau) \geq 1}} \frac{\alpha(\tau)\gamma(\tau)}{\rho(\tau)!} \left(\bar{b}_i^\top \bar{\Phi}(\tau)\right) \mathbf{f}(\tau)(y_{n-1}) h^{\rho(\tau)}, \qquad (i = 1, \ldots, s). \tag{9}$$

Now, comparing the expansions (7) and (9), there follows Proposition 2.1.

PROPOSITION 2.1. *The starting algorithm (3) has order p if this is the largest integer such that for all $i = 1, \ldots, s$, the following equations hold:*

$$1 = \alpha_i + \beta_i^\top e + \gamma_i^\top e, \tag{10}$$

$$\left(\beta_i^\top, \gamma_i^\top\right) \bar{A}\bar{\Phi}(\tau) = \tilde{b}_i^\top \tilde{\Phi}(\tau), \qquad \forall \tau \in T, \quad \text{with } 1 \leq \rho(\tau) \leq p. \tag{11}$$

REMARK 1. Although, for simplicity, we have assumed that (1) is a scalar autonomous problem, the order conditions given in Proposition 2.1 also hold for vector systems in the nonautonomous case.

REMARK 2. A proposition similar to 2.1 can be established in the case of a variable step size. Putting $h_j = t_{j+1} - t_j$ and introducing the step-size ratios $r_j = h_{j+1}/h_j$ order conditions that generalize to (10) and (11) depending on r_n and r_{n-1} can be obtained.

3. STARTING ALGORITHMS FOR THE TWO-STAGE RKG METHOD

The available parameters in the starting algorithm (4) for the two-stage RKG method are $\alpha_i \in \mathbb{R}$, $\beta_i \in \mathbb{R}^2$, and $\gamma_i \in \mathbb{R}^2$ $(i = 1, 2)$. In view of Proposition 2.1, the parameters α_i, β_i must be determined from the linear equations (11) and then α_i are uniquely determined from the consistency condition (10).

On the other hand, since $\bar{A}$ is a nonsingular matrix, it turns out to be more practical to introduce the vectors $w_i^\top = (\beta_i^\top, \gamma_i^\top)\bar{A} \in \mathbb{R}^4$ and to study the linear equations (11) in the form

$$w_i^\top \bar{\Phi}(\tau) = \tilde{b}_i^\top \tilde{\Phi}(\tau), \qquad \text{for } \tau \in T, \quad \rho(\tau) \geq 1,$$

in the unknowns $w_i \in \mathbb{R}^4$ for $i = 1, 2$, and then to come back to the original parameters β_i, γ_i.

For order three, there are four order conditions, but taking into account the simplifying assumption C(2), the third-order conditions for the trees τ_{31} and τ_{32} (here and in the following, we use for the trees, the notations of Hairer, Norsett and Wanner [8]) are equivalent and we have three independent conditions. Thus, we have a family of starting algorithms with order ≥ 3 with a free parameter. Several criteria have been considered for the choice of this parameter.

First of all, since there are two additional independent equations of order four ($\mathrm{Cond}(\tau_{41}) \Leftrightarrow \mathrm{Cond}(\tau_{42})$ and $\mathrm{Cond}(\tau_{43}) \Leftrightarrow \mathrm{Cond}(\tau_{44})$), we may use the free parameter to satisfy either of these conditions. Then, by considering the τ_{41}-condition, we obtain the method RKG2,1, with the coefficients given in Table 1.

Table 1. Coefficient starting algorithm RKG2,1.

i	α_i	$\beta_{i,1}$	$\beta_{i,2}$	$\gamma_{i,1}$	$\gamma_{i,2}$
1	$36-18\sqrt{3}$	$\frac{82-57\sqrt{3}}{2}$	$\frac{-108+71\sqrt{3}}{2}$	$\frac{4-9\sqrt{3}}{2}$	$\frac{-48+31\sqrt{3}}{2}$
2	$36+18\sqrt{3}$	$\frac{-108-71\sqrt{3}}{2}$	$\frac{82+57\sqrt{3}}{2}$	$\frac{-48-31\sqrt{3}}{2}$	$\frac{4+9\sqrt{3}}{2}$

This starting algorithm has order three, and for the local error, we have an expansion of type

$$Y_{n+1,i}^{(0)} - Y_{n+1,i} = \sum_{\rho(\tau)\geq 4} \psi_i^{[4]}(\tau)\mathbf{f}(\tau)(y_{n-1})h^4 + \mathcal{O}\left(h^5\right), \qquad (i=1,2).$$

We have computed, for $i=1,2$, the ℓ_2-norm of the coefficients of the leading error term

$$\Psi_i^{[4]} = \sqrt{\sum_{\rho(\tau)=4} \left|\psi_i^{[4]}(\tau)\right|^2}, \tag{12}$$

obtaining for the two stages the values

$$\Psi_1^{[4]}(\mathrm{RKG2,1}) = 0.015789057581792166641920557237 8,$$
$$\Psi_2^{[4]}(\mathrm{RKG2,1}) = 0.219913202813723674825027563467.$$

Similarly, by choosing the available parameter satisfying the order condition of the τ_{43}-tree, we obtain the method RKG2,2 whose coefficients are given in Table 2.

Table 2. Coefficient starting algorithm RKG2,2.

i	α_i	$\beta_{i,1}$	$\beta_{i,2}$	$\gamma_{i,1}$	$\gamma_{i,2}$
1	$24-12\sqrt{3}$	$29-20\sqrt{3}$	$-36+24\sqrt{3}$	$2-4\sqrt{3}$	$-18+12\sqrt{3}$
2	$24+12\sqrt{3}$	$-36-24\sqrt{3}$	$29+20\sqrt{3}$	$-18-12\sqrt{3}$	$2+4\sqrt{3}$

In this method, the norms of the error coefficients for the two stages are

$$\Psi_1^{[4]}(\mathrm{RKG2,2}) = 0.023536937369030486928558035024,$$
$$\Psi_2^{[4]}(\mathrm{RKG2,2}) = 0.327827247094122772182430136584.$$

Finally, for each i, we have used the free parameter of the family of order 3 to minimize the function $\Psi_i^{[4]}$ defined by (12). This leads to an elementary least squares problem and, in this way, we arrive at the method RKG2,3 given by the following coefficients.

Table 3. Coefficient starting algorithm RKG2,3.

i	α_i	$\beta_{i,1}$	$\beta_{i,2}$	$\gamma_{i,1}$	$\gamma_{i,2}$
1	$\frac{936-468\sqrt{3}}{29}$	$\frac{1081-750\sqrt{3}}{29}$	$\frac{-1404+926\sqrt{3}}{29}$	$\frac{58-126\sqrt{3}}{29}$	$\frac{-642+418\sqrt{3}}{29}$
2	$\frac{936+468\sqrt{3}}{29}$	$\frac{-1404-926\sqrt{3}}{29}$	$\frac{1081+750\sqrt{3}}{29}$	$\frac{-642-418\sqrt{3}}{29}$	$\frac{58+126\sqrt{3}}{29}$

In this case, the norms of the error coefficients for the two stages are

$$\Psi_1^{[4]}(\text{RKG2,3}) = 0.013112098633182616849362863343 6,$$
$$\Psi_2^{[4]}(\text{RKG2,3}) = 0.182627974538385212646422444984.$$

First of all, for the same method, $\Psi_2^{[4]}$ is larger than $\Psi_1^{[4]}$ because these starting algorithms are based in extrapolation of back information on the numerical solution and, clearly, the second stage goes further than the first one.

The values of $\Psi_1^{[4]}$ and $\Psi_2^{[4]}$ for the above methods show that, although the three methods are third order accurate, in a general setting, RKG2,3 is to be preferred because it has the lowest norm of the leading error term. However, for particular equations in which some elementary differentials vanish, the other starting algorithms could provide better results. In any case, since the three starting algorithms have the same order and one step of the functional iteration that is commonly used in the solution of stage equations increases the order of accuracy by one, one cannot expect that RKG2,3 allows us to reduce significantly, with respect to the other third-order algorithms, the average of number iterations per step.

4. STARTING ALGORITHMS FOR THE THREE-STAGE RKG METHOD

In this case, we have seven free parameters $\alpha_i \in \mathbb{R}$, $\beta_i \in \mathbb{R}^3$, and $\gamma_i \in \mathbb{R}^3$ $(i = 1, 2, 3)$ for each stage. On the other hand, taking into account that the three-stage RKG method satisfies the C(3) simplifying condition, there are seven independent conditions to be satisfied for order five. However, such a set of seven linear equations in the seven parameters turns out to be incompatible and we cannot get a starting algorithm of order five. In view of this, we have considered methods of order four that satisfy some additional conditions related to the higher-order error terms. More precisely, we proceed in the following way.

(1) Since there are five linearly independent conditions of order four, we have taken two free parameters u, v and constructed, for each stage, a family of starting algorithms of order four in which all the coefficients α_i, $\beta_{i,1}$, $\beta_{i,2}$, $\beta_{i,3}$, $\gamma_{i,1}$, $\gamma_{i,2}$, $\gamma_{i,3}$ depend linearly on u and v.

(2) By substituting these expressions of the coefficients into the two independent conditions of order five (τ_{51}, τ_{56}), we obtain two linear equations in the parameters which are parallel straight lines in the (u, v)-plane. Thus, they cannot be satisfied simultaneously and then we have decided to choose u and v so that they minimize the ℓ_2 norm of the coefficients of the terms of order five. This leaves one free parameter.

(3) Furthermore, we proceed similarly with the terms of order six, i.e., using the free parameter so that we minimize the ℓ_2 norm of the coefficients of the terms of order six.

(4) The above requirements (2) and (3) lead to a unique solution for the parameters u and v, and therefore, for the method.

After these calculations, the resulting method RKG3,1 has the following coefficients:

$$\alpha_1 = \frac{310116078388 - 77043925428\sqrt{15}}{485094169},$$

$$\alpha_2 = \frac{13920180178}{69299167},$$
$$\alpha_3 = \frac{310116078388 + 77043925428\sqrt{15}}{485094169}.$$

Table 4. Coefficient starting algorithm RKG3,1.

β_1	β_2	β_3
$\frac{-1183989608707+290480477045\sqrt{15}}{1455282507}$	$\frac{-1332692895\sqrt{15}}{138598334} - \frac{124575062795}{415795002}$	$-\frac{1553508840610+389407014221\sqrt{15}}{1455282507}$
$\frac{1260504227504-313185680200\sqrt{15}}{1455282507}$	$\frac{56725317833}{207897501}$	$\frac{1260504227504+313185680200\sqrt{15}}{1455282507}$
$\frac{-1553508840610+389407014221\sqrt{15}}{1455282507}$	$-\frac{124575062795}{415795002} + \frac{1332692895\sqrt{15}}{138598334}$	$-\frac{1183989608707+290480477045\sqrt{15}}{1455282507}$

γ_1	γ_2	γ_3
$\frac{3764}{217} + \frac{24327445\sqrt{15}}{1455282507}$	$\frac{10615381635+2444034375\sqrt{15}}{138598334}$	$\frac{197782732080}{485094169} + \frac{152246600771\sqrt{15}}{1455282507}$
$\frac{-73576}{1519} + \frac{52144\sqrt{15}}{4557}$	$-\frac{5792}{217}$	$-\frac{73576}{1519} - \frac{52144\sqrt{15}}{4557}$
$\frac{197782732080}{485094169} - \frac{152246600771\sqrt{15}}{1455282507}$	$\frac{10615381635-2444034375\sqrt{15}}{138598334}$	$\frac{3764}{217} - \frac{24327445\sqrt{15}}{1455282507}$

5. NUMERICAL EXPERIMENTS

In this section, we present some numerical experiments comparing the behaviour of the new starting algorithms with the standard starting algorithm based in the collocation polynomial in the stages of the previous step [7, Section 4]. As a first test problem, we consider the well-known two-dimensional Kepler problem whose Hamiltonian function is given by

$$H(p,q) = \frac{1}{2}\left(p_1^2 + p_2^2\right) - \frac{1}{\sqrt{q_1^2 + q_2^2}}, \tag{13}$$

with initial conditions

$$p_1(0) = 0, \qquad p_2(0) = \sqrt{\frac{1+e}{1-e}}, \qquad q_1(0) = 1 - e, \qquad q_2(0) = 0. \tag{14}$$

For $e \in [0,1)$, the solution of Hamilton's equations corresponding to (13) with initial conditions (14) is periodic with period 2π and the orbit in the (q_1, q_2)-plane is an ellipse with eccentricity e.

Several Poincaré regularizing transformations have been suggested in the literature with the form

$$\frac{dt}{d\tau} = g(q) = \left(q_1^2 + q_2^2\right)^r,$$

where r is a positive fixed constant. In the numerical experiments presented here, we have chosen the value $r = 1$ following the suggestions of [2,5], then the new independent variable τ is the so-called true anomaly in the two body problem.

For a given set of initial conditions (14), the modified Hamiltonian in the new independent variable τ is

$$\hat{H}(p,q) = g(q)[H(p,q) - H(p(0),q(0))],$$

therefore, in our numerical experiments, we have considered Hamilton's equations with respect to $\hat{H}(p,q)$ with τ as an independent variable and the initial conditions given by (14).

We have implemented the two- and three-stage RKG methods with a fixed step size and used functional iteration for the solution of stage equations and different starting algorithms. The iterations have been carried out up to the roundoff level.

For the fourth-order RKG method, we will denote by RKG2,1, RKG2,2, RKG2,3, the above starting algorithms of order three for the two-stage RKG method given in Tables 1, 2, and 3, respectively, and by RKG2,Lag the starting algorithm of order two given by the collocation polynomial in the previous step [7, Section 3].

For the three-stage RKG method, we will denote by RKG3,1 the starting algorithm of order four given in Table 4 and by RKG3,Lag the starting algorithm of order three corresponding to the collocation polynomial on the stages of the previous step [7, Section 4].

Our aim is to measure the number of fixed-point iterations required to solve the stage equations by using either of the above starting algorithms. Since the problem is periodic, it is enough to compute the average of iterations per step in one period. Observe that all starting algorithms considered here do not require additional function evaluations.

In Table 5, we present the average of iterations per step in one period for the two-stage RK-Gauss method when $e = 0.9$, and the step sizes specified.

Table 5. Iteration/step, $e = 0.9$.

Steps	RKG2,1	RKG2,2	RKG2,3	RKG2,Lag
128	7.29	7.31	7.23	8.10
256	5.62	5.67	5.61	6.34
512	4.40	4.47	4.43	5.35
1024	3.57	3.70	3.59	4.43
2048	2.98	3.06	2.99	3.85
4096	2.44	2.47	2.44	3.30
8192	2.05	2.10	2.03	3.00

In Table 6, we show the results for the three-stage RKG method.

Table 6. Iteration/step, $e = 0.9$.

Steps	RKG3,1	RKG,Lag
64	8.06	9.05
128	5.83	6.80
256	4.45	5.41
512	3.47	4.45
1024	2.61	3.64
2048	2.06	3.04

From the above results, it follows that the new starting algorithms for the two- and the three-stages RKG methods employ around one fixed iteration less than their corresponding standard algorithms to achieve the desired convergence. In addition, among the algorithms for the two-stage RKG, the RKG2,1 and RKG2,3 show a slightly better behaviour. This fact has been confirmed by other numerical experiments not presented here and can be due to the fact that $\Psi_1^{[4]}$ and $\Psi_2^{[4]}$ for the RKG2,2 are slightly larger than for RKG2,1 and RKG2,3.

Next, in Table 7, we present the numerical results obtained for the two body problem with a higher eccentricity $e = 0.99$. Although the use of the true anomaly as Poincaré regularizing

variable improves the convergence behaviour of the fixed-point iteration, this problem, due to its high eccentricity, poses more difficulties for convergence of the iterative scheme than the case $e = 0.9$.

Table 7. Iteration/step, $e = 0.99$.

Steps	RKG2,1	RKG2,2	RKG2,3	RKG2,Lag
128	8.74	8.98	8.72	**
256	6.51	6.55	6.50	**
512	5.04	5.13	5.06	5.96
1024	4.08	4.27	4.16	4.89
2048	3.36	3.42	3.39	4.23
4096	2.81	2.82	2.81	3.64
8192	2.22	2.32	2.26	3.16

Here, the stars indicate that with the corresponding starting values, the iterative scheme does not converge. This means that the new starting algorithms are more robust than the standard collocation for the convergence of the fixed-point iteration. This remarkable fact also holds for the RKG3,1 and for other numerical examples, particularly when the step size of integration is not small.

The next example presented here is the so-called outer solar system which appears as problem C5 in [9]. This problem simulates the motion of the five outer planets around the Sun under the assumption that the Sun concentrates the mass of the inner planets. Then, the Sun and the outer planets are considered as point masses moving under their mutual gravitational forces. By using heliocentric coordinates and taking into account the six integrals of the linear momentum, the original system can be reduced to a set of five second-order vector equations (equivalent to 30 first order equations), each of these vectors is the position of an outer planet with respect to the Sun. With these position-velocities variables, the system is not Hamiltonian, but using a linear combination of velocities, the system can be written in Hamiltonian form. However, since a linear transformation (even noncanonical), transforms linearly, the starting values and the iterates of the fixed-point iteration, we have considered the problem in the usual position-velocity variables.

We have taken an integration interval of about two times the period of Jupiter and no regularizing transformation has been employed due to the fact that the eccentricity of the orbits of outer planets is small. To test the accuracy of the numerical integration, we have used the four integrals of energy and angular momentum computing its values along the numerical solution. In Table 9, we present the results obtained for the two stage RKG method.

Table 9. Iteration/step, C5 problem.

Steps	RKG2,1	RKG2,2	RKG2,3	RKG2,Lag
64	10.77	10.80	10.70	11.97
128	8.03	7.75	8.03	9.02
256	6.02	5.75	6.02	7.01
512	5.01	4.90	5.01	6.00
1024	4.00	3.81	4.00	5.00
2048	3.00	3.00	3.00	4.00
4096	3.00	3.00	3.00	4.00
8192	2.00	2.00	2.00	3.00

From Table 9, it follows that the behaviour of the new starting algorithms for this problem with dimension 30 is very similar to the case of the two-body problem, i.e., the number of fixed-point iterations is reduced by one without extra function evaluations. It must be noticed that in the C5-problem, since the orbits of the outer planets are close to the circular case, the number of

iterations remains constant along the integration (except probably in the first and second steps). Thus, values such as 6.02 indicate that, except for the initial steps, the fixed-point iteration has used six iterations per step. Similar results have been obtained for the three-stage method.

6. CONCLUSION

New algorithms that provide starting values for the iterative solution of stage equations in two- and three-step RKG methods have been proposed. The new algorithms (without extra computational cost) allow us to reduce (on average) the number of fixed-point iterations by one with respect to the standard collocation algorithm. Moreover, they are also more robust than the standard ones.

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